

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
 Data File : BF133882.D
 Acq On : 21 Jun 2023 21:10
 Operator : CG\JU
 Sample : 03296-07
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSIT-R-01

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133882.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	4	9	20	rVB	422638	557818	26.70%	2.742%
2	2.257	24	29	38	rVB2	27429	42418	2.03%	0.209%
3	5.093	506	511	525	rVB	730966	897699	42.98%	4.413%
4	5.492	575	579	583	rBV	1889884	1876068	89.81%	9.222%
5	5.881	641	645	651	rBV	48960	46071	2.21%	0.226%
6	6.492	745	749	759	rBV	1803452	1859292	89.01%	9.139%
7	6.857	808	811	815	rBV	722005	613809	29.38%	3.017%
8	7.422	903	907	910	rBV	1388225	1173072	56.16%	5.766%
9	8.139	1025	1029	1032	rBV	884426	682278	32.66%	3.354%
10	9.216	1208	1212	1215	rBV	2504259	1914001	91.63%	9.408%
11	9.757	1301	1304	1307	rBV	32831	26686	1.28%	0.131%
12	9.898	1324	1328	1331	rBV	709528	610552	29.23%	3.001%
13	9.927	1331	1333	1337	rVB	39874	30782	1.47%	0.151%
14	10.104	1358	1363	1367	rBV2	24548	26427	1.27%	0.130%
15	10.445	1417	1421	1427	rBV2	26888	26738	1.28%	0.131%
16	10.610	1445	1449	1453	rBV	127650	113067	5.41%	0.556%
17	10.686	1458	1462	1469	rBV	1259267	1108212	53.05%	5.447%
18	10.816	1479	1484	1488	rVB4	20882	30336	1.45%	0.149%
19	11.392	1578	1582	1584	rBV	746502	686395	32.86%	3.374%
20	11.416	1584	1586	1589	rVV	319340	258547	12.38%	1.271%
21	11.463	1589	1594	1598	rVB	89216	82838	3.97%	0.407%
22	11.622	1615	1621	1627	rBV2	39914	57284	2.74%	0.282%
23	11.892	1663	1667	1669	rBV	53484	53967	2.58%	0.265%
24	11.921	1669	1672	1676	rVV	299315	276295	13.23%	1.358%
25	12.004	1683	1686	1689	rBV	78595	90200	4.32%	0.443%
26	12.098	1695	1702	1705	rBV6	20415	39899	1.91%	0.196%
27	12.192	1715	1718	1720	rBV	37959	30615	1.47%	0.150%
28	12.216	1720	1722	1725	rVB	40082	35818	1.71%	0.176%
29	12.445	1758	1761	1765	rBV	42728	55571	2.66%	0.273%
30	12.533	1773	1776	1781	rVB2	45186	42529	2.04%	0.209%
31	12.610	1785	1789	1794	rVV	752755	641173	30.69%	3.152%
32	12.710	1802	1806	1809	rBV2	86148	96350	4.61%	0.474%
33	12.839	1822	1828	1834	rBV	646294	715509	34.25%	3.517%
34	12.886	1834	1836	1841	rVB2	32210	41618	1.99%	0.205%
35	12.986	1849	1853	1860	rVB	2399210	2088874	100.00%	10.268%
36	13.057	1861	1865	1869	rBV3	48238	79575	3.81%	0.391%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
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37	13.151	1877	1881	1882	rBV3	37609	47328	2.27%	0.233%
38	13.168	1882	1884	1887	rVB	85461	83900	4.02%	0.412%
39	13.239	1894	1896	1898	rVB	62986	45700	2.19%	0.225%
40	13.274	1898	1902	1905	rBV2	70687	73779	3.53%	0.363%
41	13.368	1915	1918	1921	rBV	40130	34197	1.64%	0.168%
42	13.398	1921	1923	1927	rBV2	37417	38853	1.86%	0.191%
43	13.563	1947	1951	1955	rBV6	34935	66471	3.18%	0.327%
44	13.680	1969	1971	1976	rVB	65738	68424	3.28%	0.336%
45	13.798	1988	1991	1993	rBV3	48107	51336	2.46%	0.252%
46	13.821	1993	1995	1997	rVV	44481	34236	1.64%	0.168%
47	13.845	1997	1999	2004	rVV2	37524	50653	2.42%	0.249%
48	13.898	2004	2008	2018	rVV3	183070	288071	13.79%	1.416%
49	14.045	2027	2033	2036	rBV2	714115	1029056	49.26%	5.058%
50	14.074	2036	2038	2043	rVB	320324	270647	12.96%	1.330%
51	14.151	2049	2051	2054	rVB2	56818	50439	2.41%	0.248%
52	15.110	2210	2214	2218	rBV	216958	352616	16.88%	1.733%
53	15.427	2265	2268	2274	rVB	120689	153280	7.34%	0.753%
54	15.492	2275	2279	2285	rVB	165699	206892	9.90%	1.017%
55	15.557	2286	2290	2294	rBV	297169	389403	18.64%	1.914%

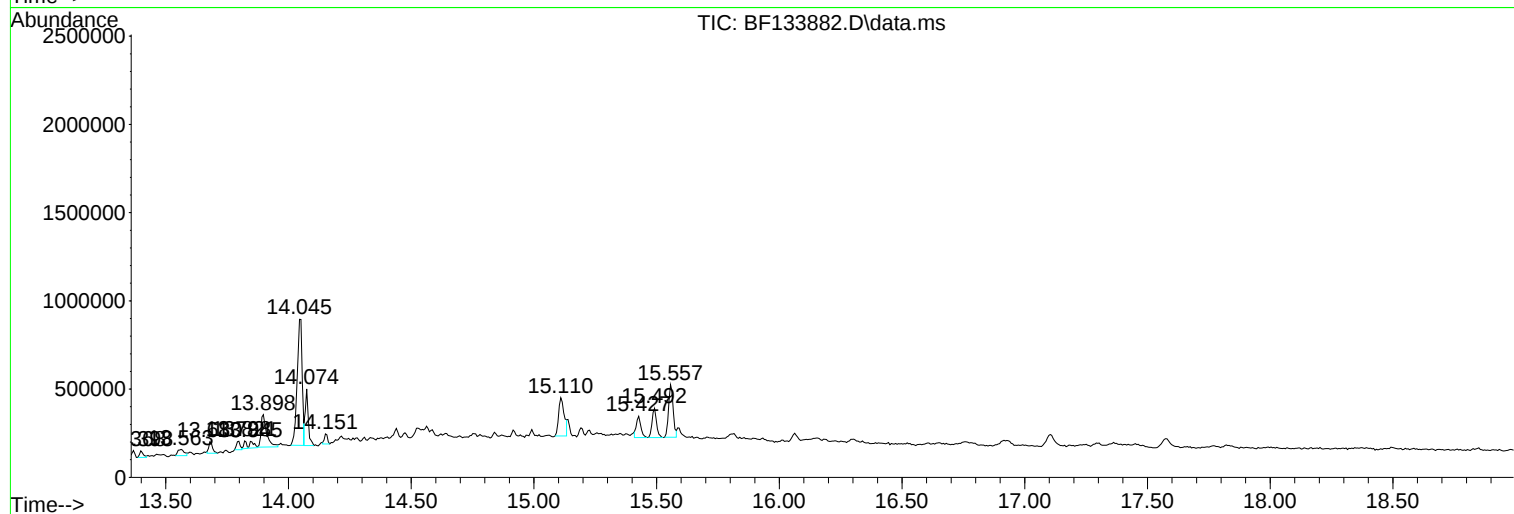
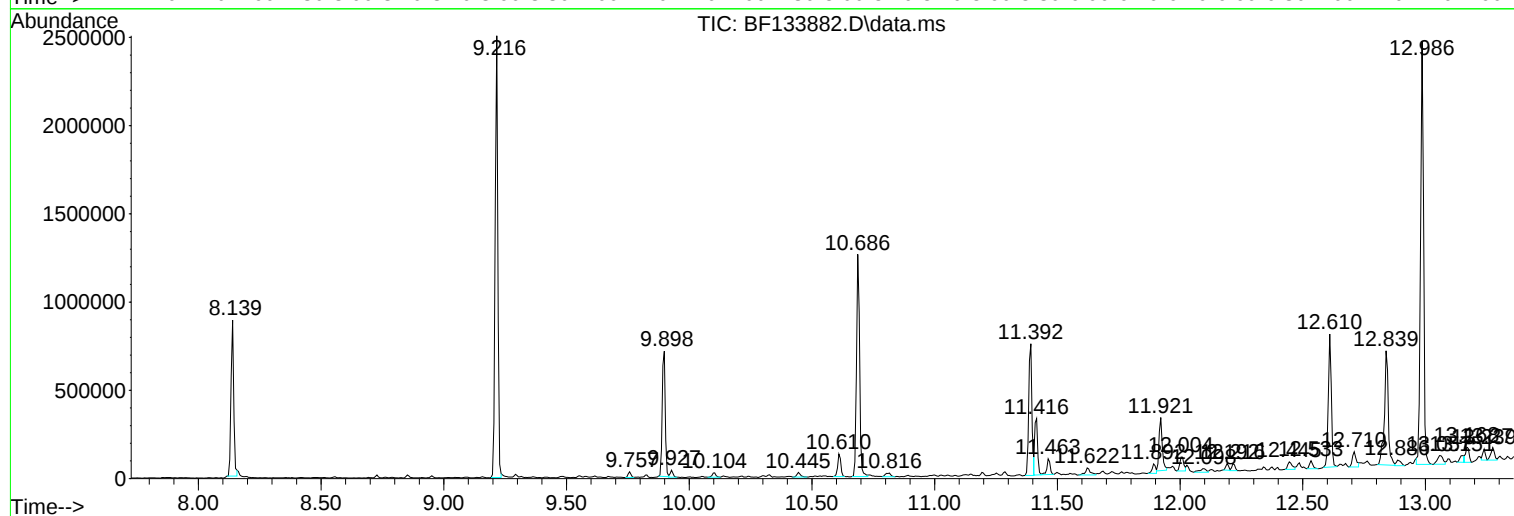
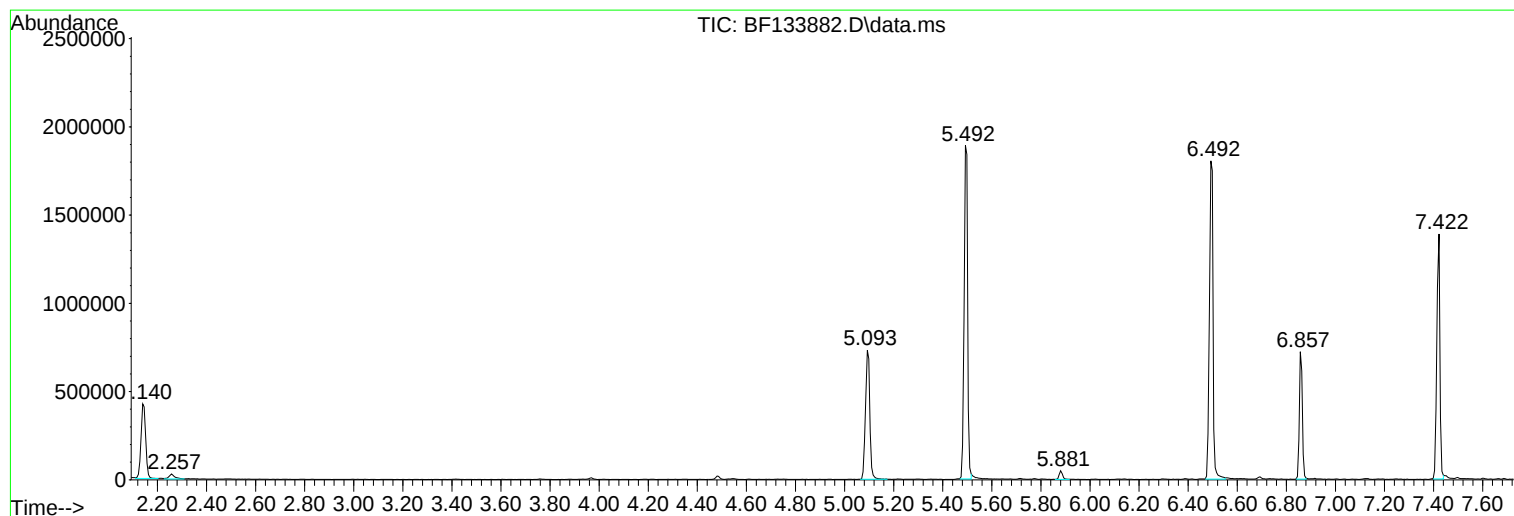
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Operator : CG\JU
Sample : 03296-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-R-01

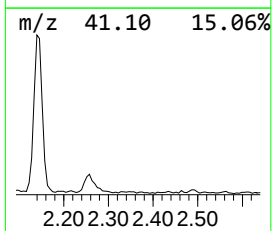
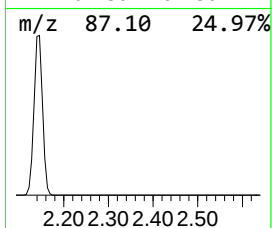
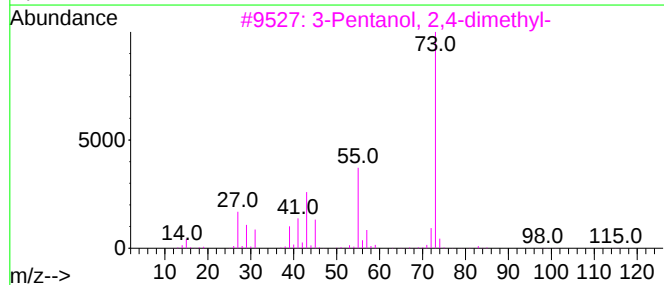
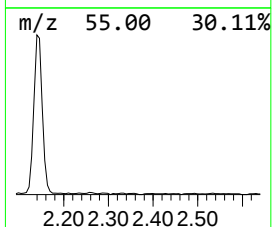
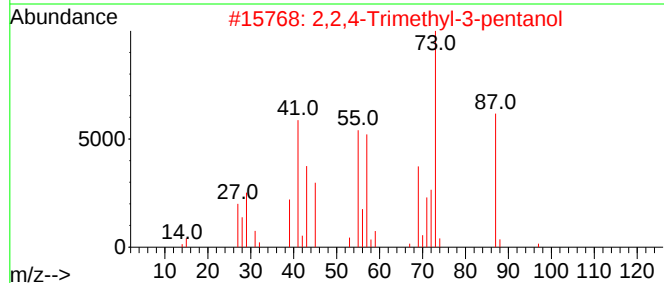
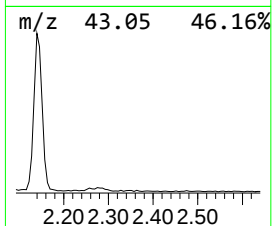
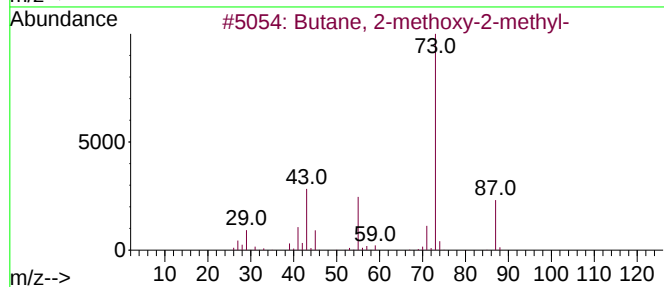
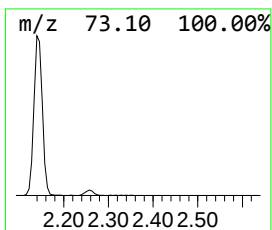
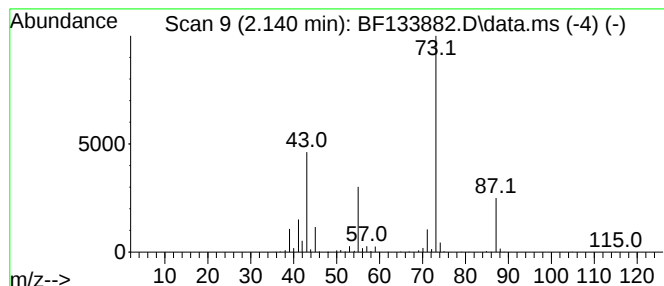
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	18.18 ng	557818	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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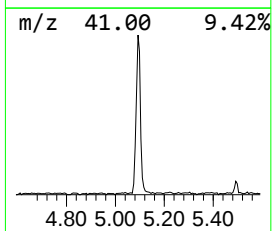
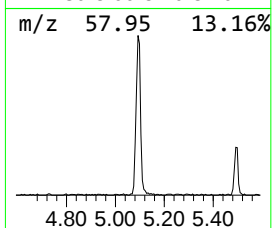
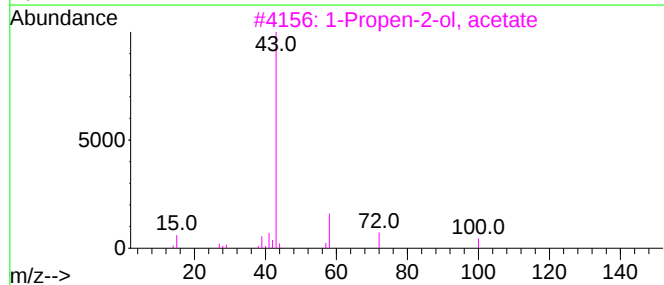
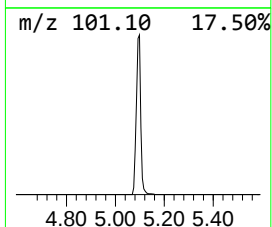
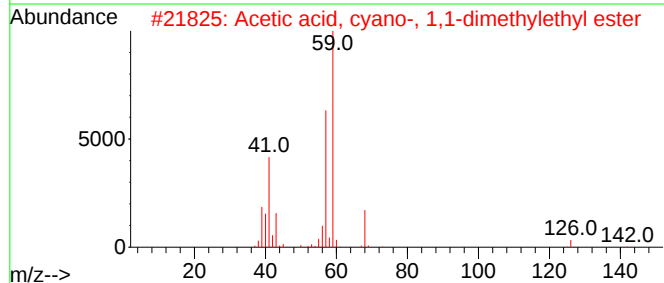
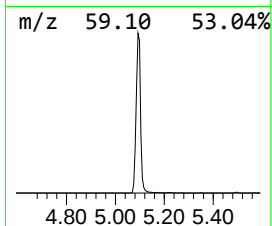
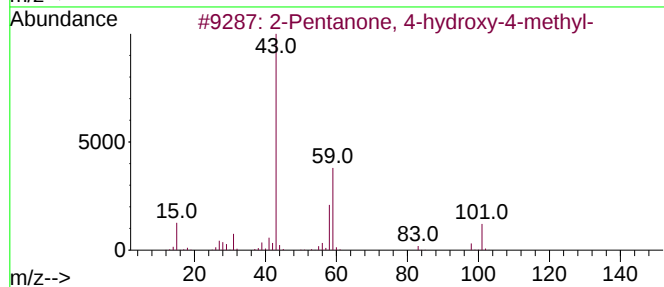
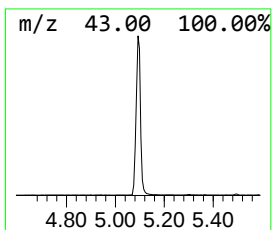
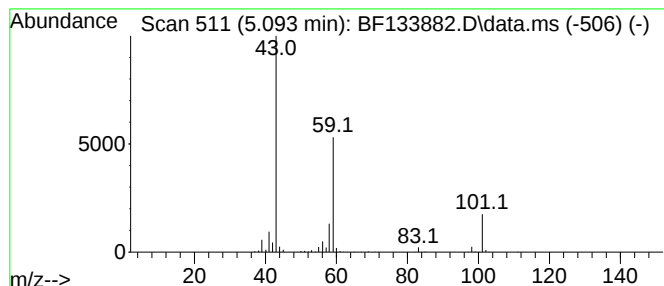
Instrument :
BNA_F
ClientSampleId :
COMPOSIT-R-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.093	29.25 ng	897699	1,4-Dichlorobenzene-d4	6.857	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

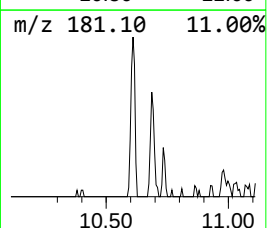
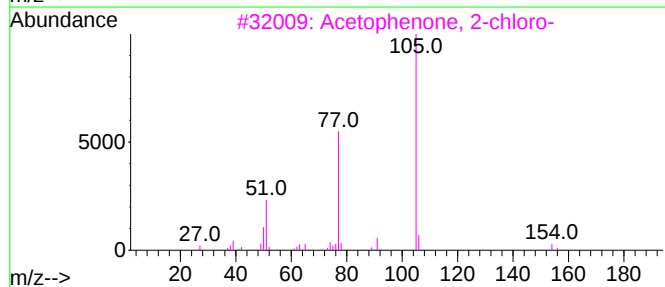
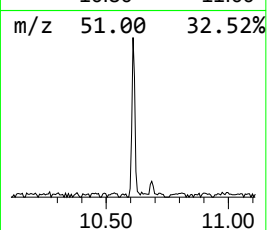
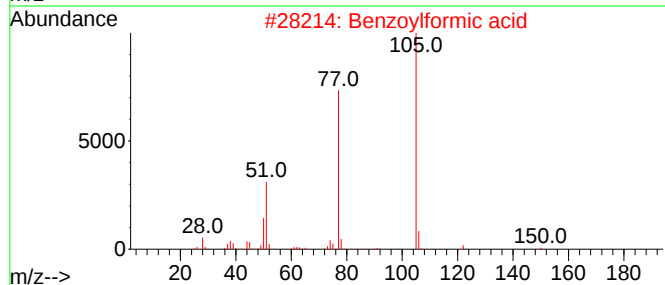
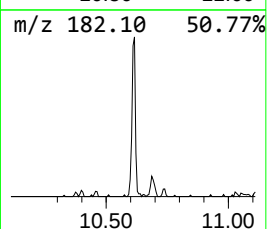
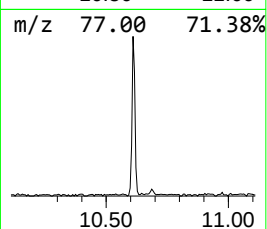
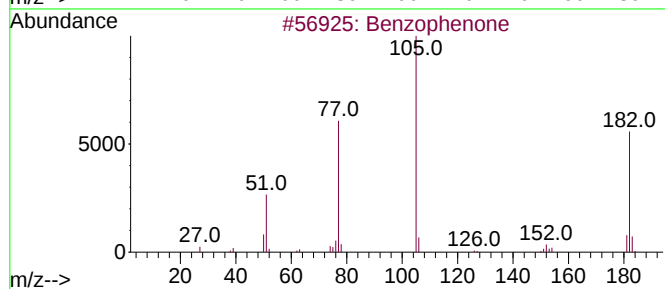
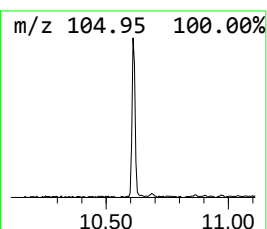
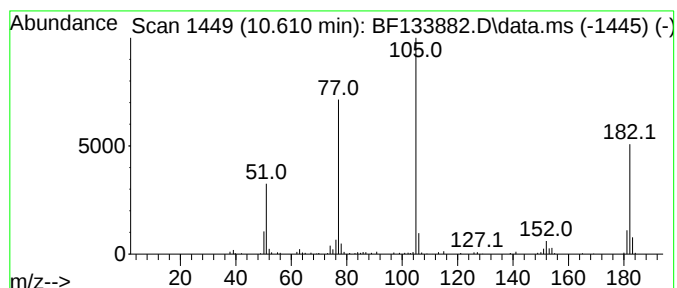
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	3.70 ng	113067	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzoylformic acid	150	C8H6O3	000611-73-4	49
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
5			Benzenebutanoic acid, .gamma.-ox...	192	C11H12O3	025333-24-8	47



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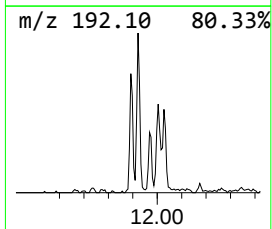
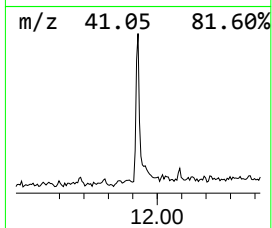
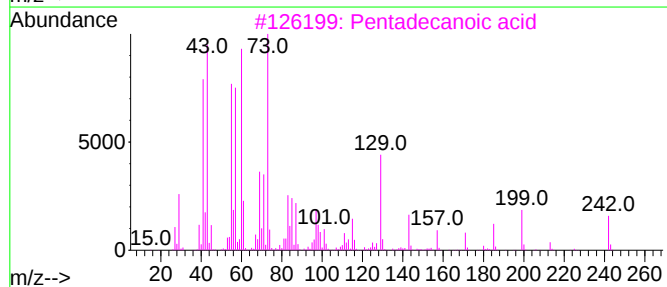
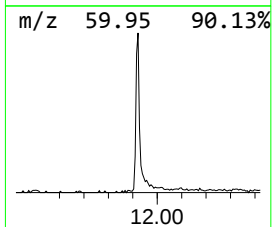
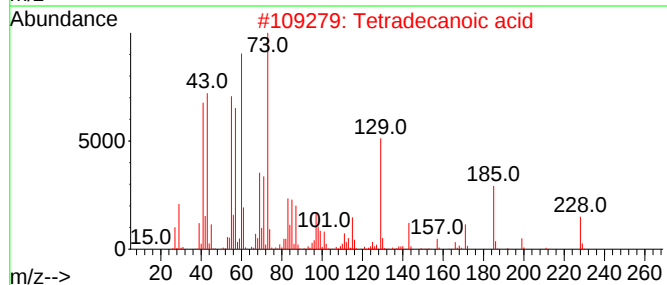
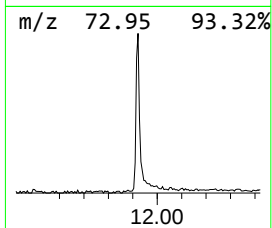
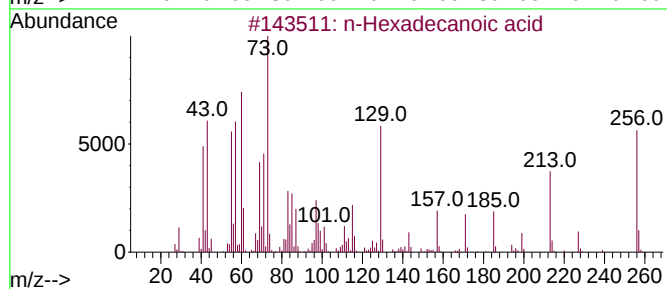
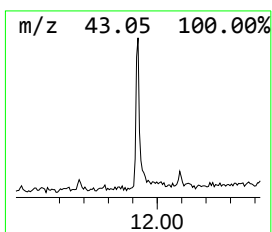
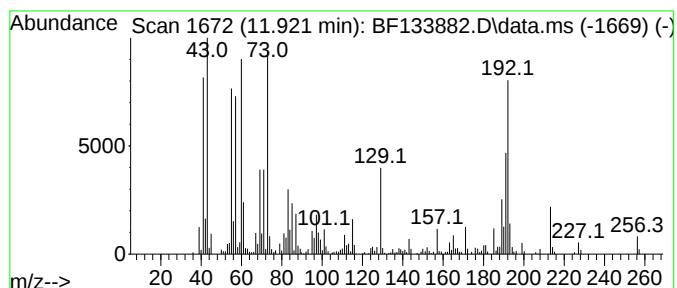
Instrument :
BNA_F
ClientSampleId :
COMPOSIT-R-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.922	8.05 ng	276295	Phenanthrene-d10		11.392	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	95
2	Tetradecanoic acid		228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	70
4	Phenanthrene, 2-methyl-		192	C15H12	002531-84-2	68
5	Phenanthrene, 4-methyl-		192	C15H12	000832-64-4	64



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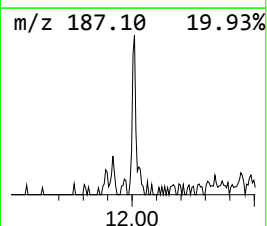
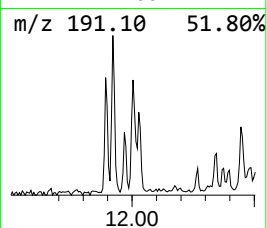
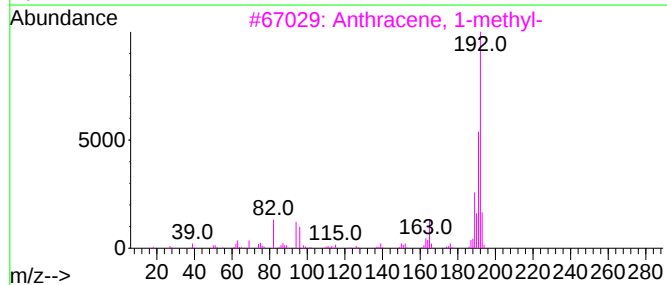
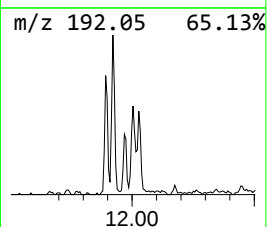
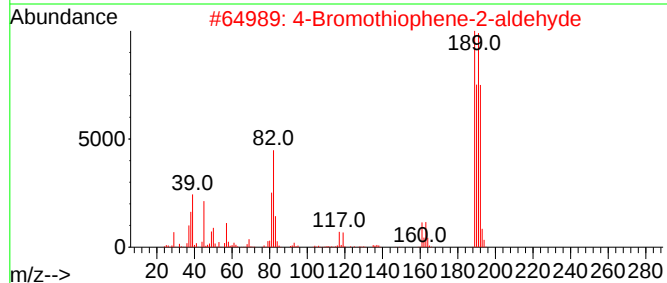
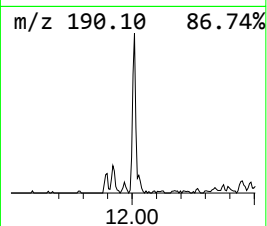
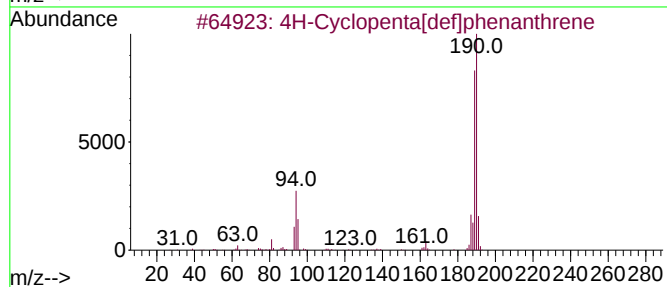
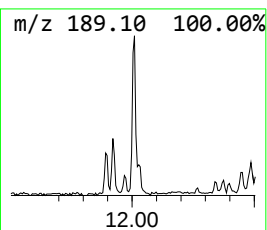
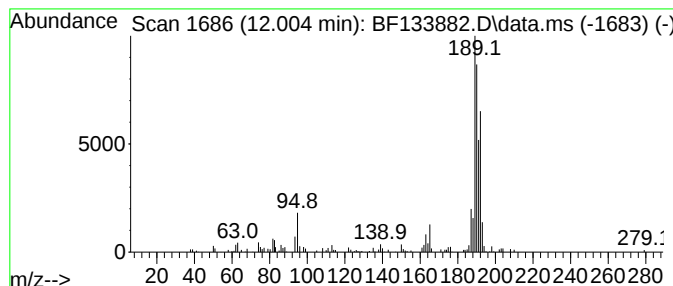
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ClientSampleId :
COMPOSIT-R-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.004	2.63 ng	90200	Phenanthrene-d10		11.392	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene		190	C15H10	000203-64-5	70
2	4-Bromothiophene-2-aldehyde		190	C5H3BrOS	018791-75-8	58
3	Anthracene, 1-methyl-		192	C15H12	000610-48-0	30
4	8,9-Dihydrocyclopenta[def]phenan...		192	C15H12	027410-55-5	30
5	Cyclohexanone, 2-(2-furanylmethy...		190	C12H14O2	056053-07-7	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133882.D
Acq On : 21 Jun 2023 21:10
Operator : CG\JU
Sample : 03296-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-R-01

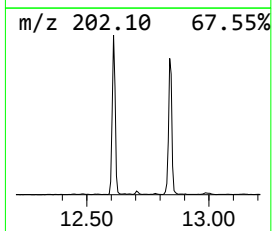
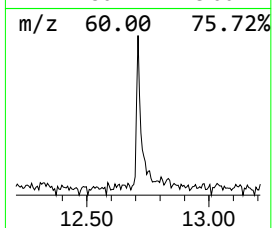
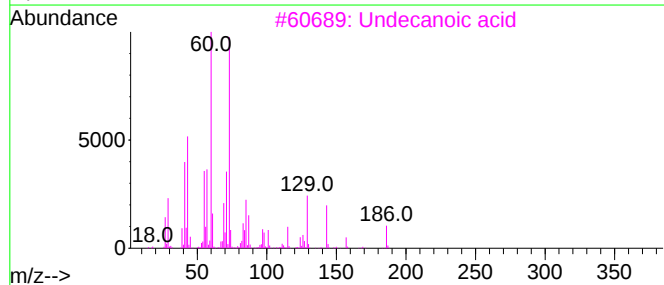
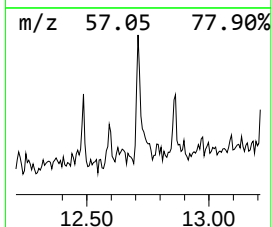
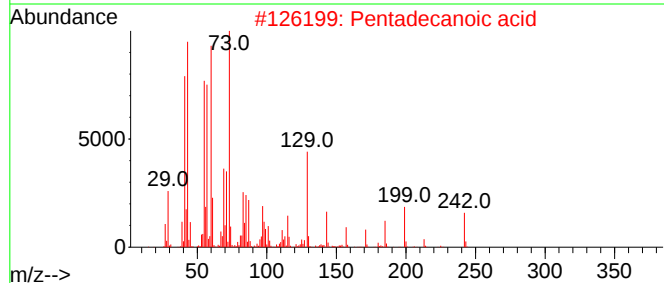
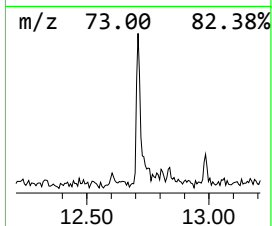
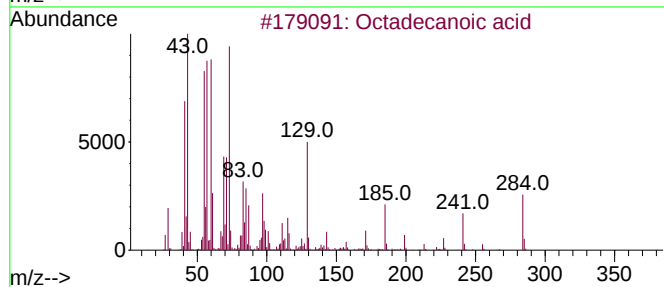
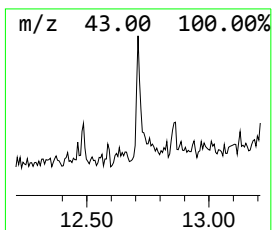
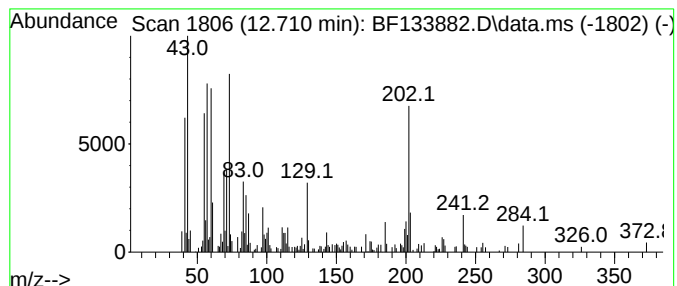
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	2.81 ng	96350	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Undecanoic acid	186	C11H22O2	000112-37-8	64
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133882.D
Acq On : 21 Jun 2023 21:10
Operator : CG\JU
Sample : 03296-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-R-01

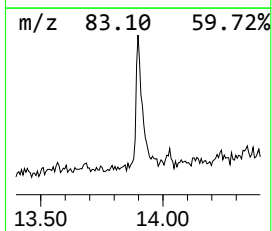
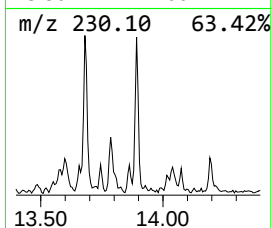
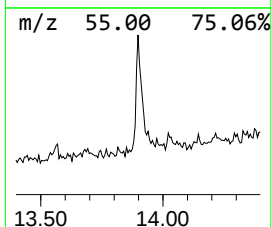
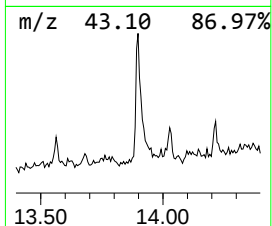
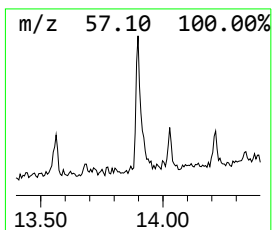
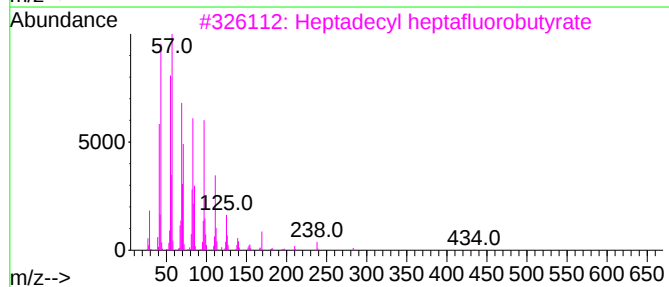
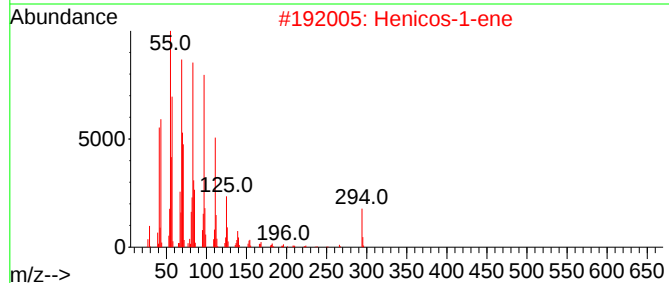
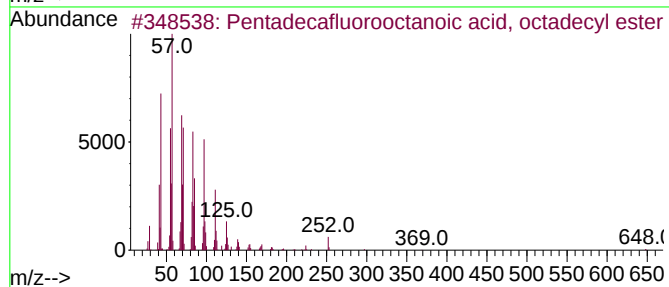
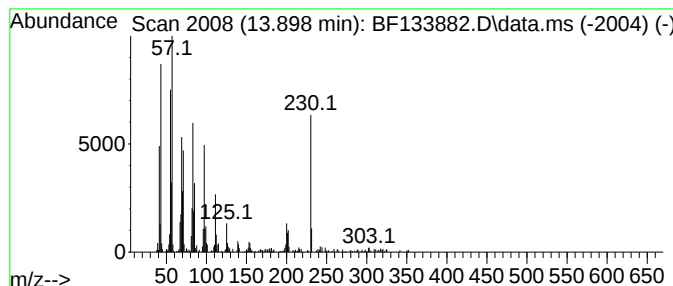
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	5.60 ng	288071	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	86
2			Henicos-1-ene	294	C21H42	001599-68-4	78
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	70
4			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	70
5			17-Pentatriacontene	491	C35H70	006971-40-0	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133882.D
Acq On : 21 Jun 2023 21:10
Operator : CG\JU
Sample : 03296-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-R-01

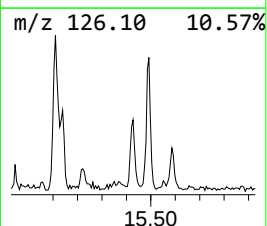
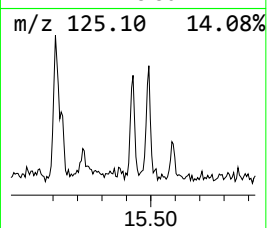
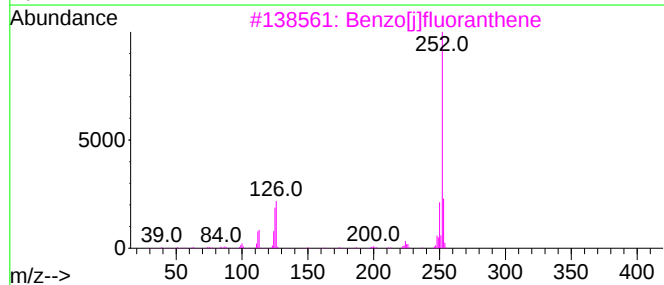
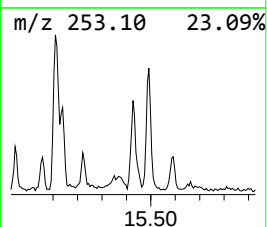
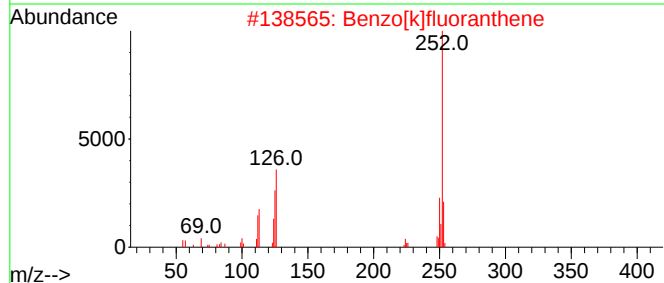
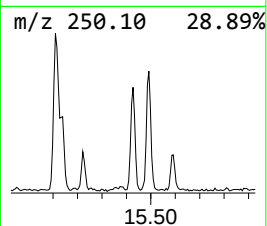
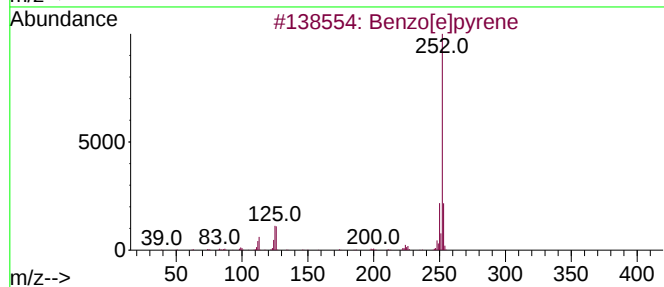
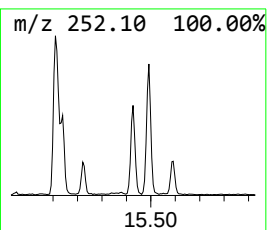
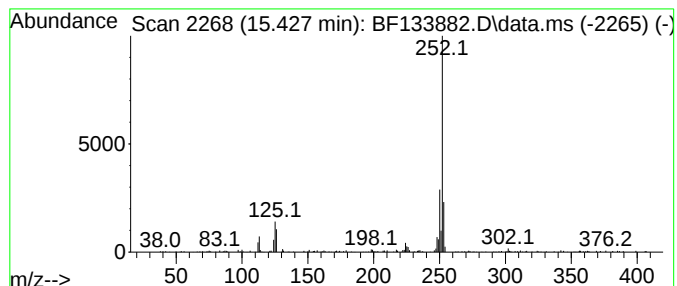
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.427	7.87 ng	153280	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3			Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
5			Perylene	252	C20H12	000198-55-0	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133882.D
Acq On : 21 Jun 2023 21:10
Operator : CG\JU
Sample : 03296-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-R-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.140	18.2	ng	557818	1	6.857	613809	20.0
2-Pentanone, 4-...	5.093	29.3	ng	897699	1	6.857	613809	20.0
Benzophenone	10.610	3.7	ng	113067	3	9.898	610552	20.0
n-Hexadecanoic ...	11.922	8.1	ng	276295	4	11.392	686395	20.0
4H-Cyclopenta[d...]	12.004	2.6	ng	90200	4	11.392	686395	20.0
Octadecanoic acid	12.710	2.8	ng	96350	4	11.392	686395	20.0
Pentadecafluoro...	13.898	5.6	ng	288071	5	14.051	1029060	20.0
Benzo[e]pyrene	15.427	7.9	ng	153280	6	15.557	389403	20.0